Oral presentation

Stabilizing low-symmetry based functions of materials at high temperature

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Symmetry breaking is pivotal for controlling ferroic functions in materials, such as ferroelectric, ferromagnetic or ferroelastic [1, 2], which enables applications in sensors, memories, transducers or actuators [3]. Commonly, ferroic phases emerge from descendant symmetry-breaking. Indeed, the laws of thermodynamics dictate that the ordered low entropy ferroic phase forms at low temperature, which limits practical applications. Some rare examples of ascendant symmetry breaking have been observed, but the driving force remains often unclear. In this communication I pretend to show how an electronic spin state change strongly coupled with a symmetry-breaking phase transitions can open a promising avenue of stabilization of low symmetry functions at high temperature.

In this regard, a detailed analysis on the anomalous ferroelastic phase transition of the spin-crossover material [Fe^{II}(PM-PEA)$_2$(NCS)$_2$] is going to be presented[4]. This mononuclear complex undergoes an unusual transformation from a low-spin high-symmetry phase ***LShs*** (*Pccn*) to a high-spin low-symmetry phase ***HSls*** (*$P2_1/c$*) by temperature rising. Information extracted from single-crystal X-Ray diffraction measurements will provide detailed insight into the characteristic features associated to the symmetry- breaking and spin-crossover phenomena. In addition, combination of DFT calculations and a mathematical model based on Landau's theory will show how the thermal change of spin state drives a ferroelastic phase transition through a coupled Jahn-Teller distortion. The large entropy gain associated with the electronic bi-stability overcomes the entropy cost due to symmetry-breaking in this molecular material. This result may pave the way for applications of multifunctional low-symmetry materials operating at room temperature.

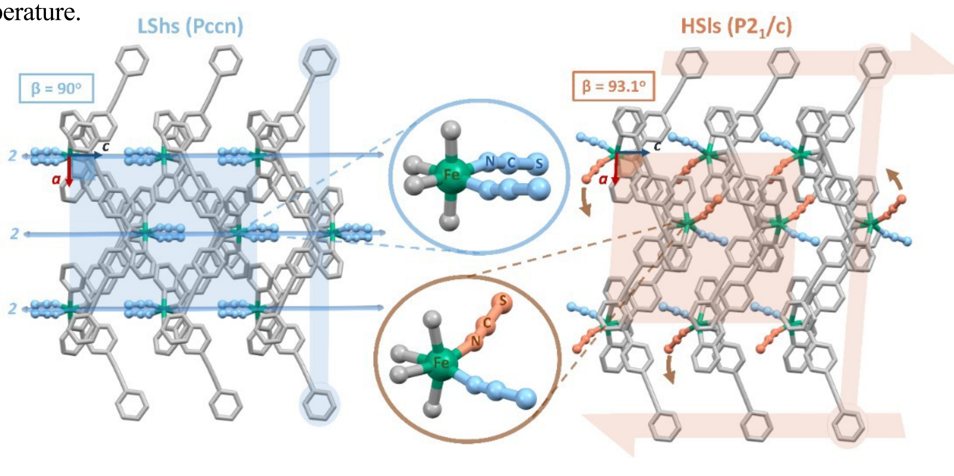

Figure 1. Ferroelastic phase transition between the low-spin high-symmetry phase (***LShs***) and the high-spin low-symmetry phase (***HSls***) in [Fe^{II}(PM- PEA)$_2$(NCS)$_2$]. The loss of 2-fold axis, shear movement of molecular layers and asymmetric torsion of NCS groups upon the phase transition are highlighted.

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The authors acknowledge the financial support from the Agence Nationale de la Recherche under the grants ANR-19-CE30-0004 ELECTROPHONE and ANR-19-CE07-0027 SMAC. F. J. V.-M. acknowledges the support of the European Social Fund(ESF) and Generalitat Valenciana for his postdoctoral fellowship (APOSTD/2021/359) and Région Bretagne (BIENVENÜE-MSCA COFUND nº 899546).